

Spin Density Transfer from Guest to Host in Endohedral Heterofullerene Dimers

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Table S1 The energy difference and energy of cis and trans form of $(C_{59}N)_2$, $(C_{59}B)_2$ and $(C_{59}B-C_{59}N)$.

System	Cis (Hartree)	Trans (Hartree)	Energy Difference (kcal/mol)
$(C_{59}N)_2$	-4606.8155971	-4606.8290581	-8.45
$(C_{59}B)_2$	-4547.02252	-4547.032562	-6.30
$C_{59}B-C_{59}N$	-4576.9312008	-4576.9314726	-0.17

Table S2 The calculated parameters of $(B@C_{60})_2$ at B3LYP-GD2/6-311G* level

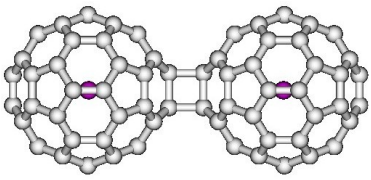
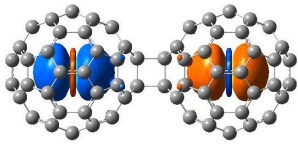
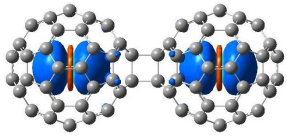
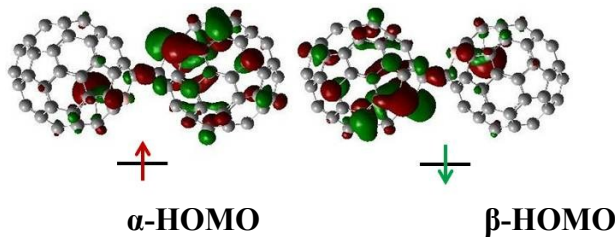
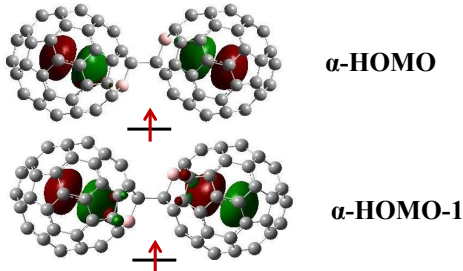
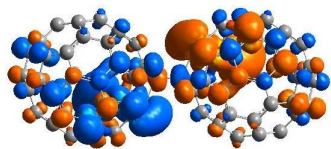
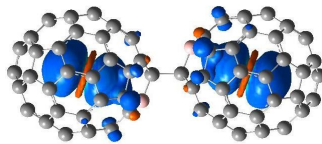
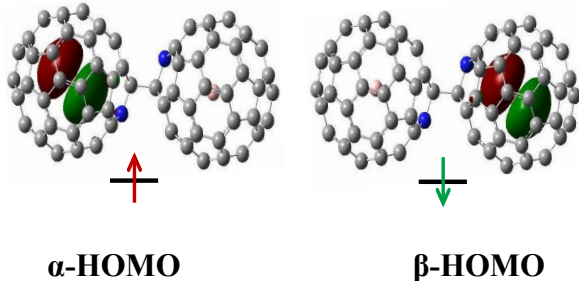
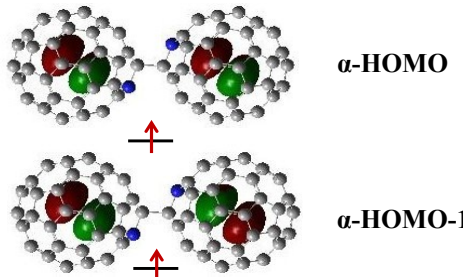
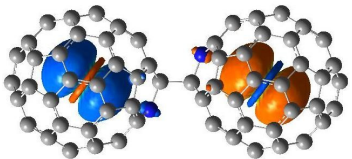
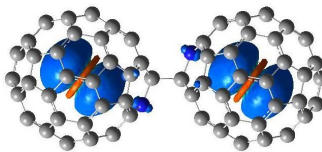
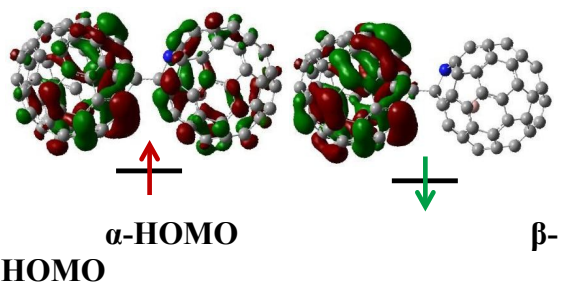
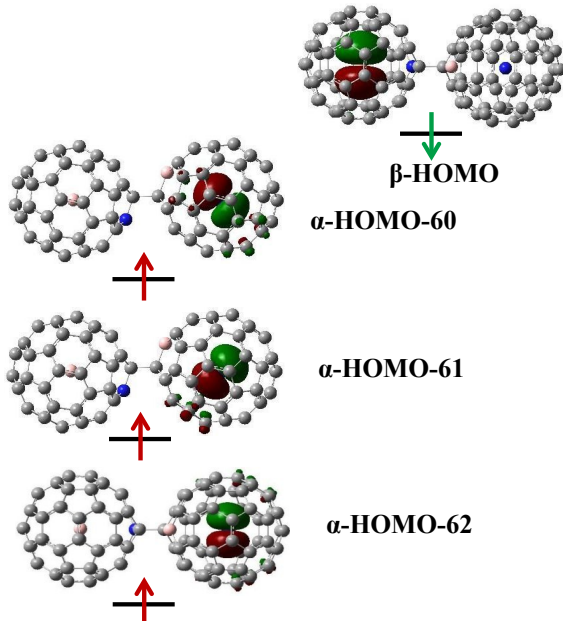
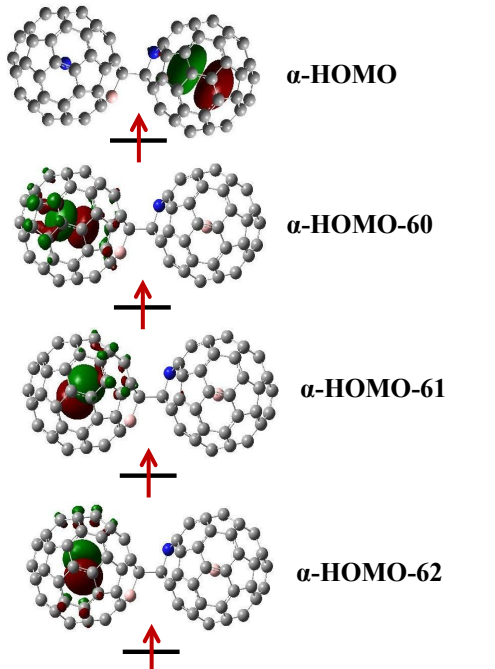
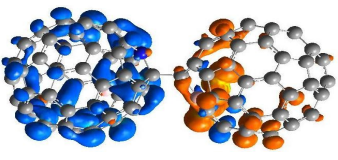
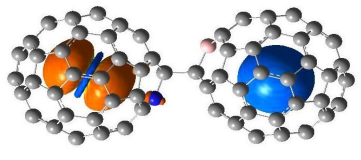
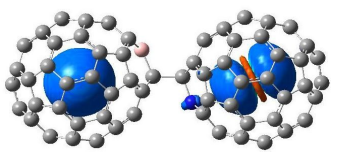
	Multiplicity	 $(B@C_{60})_2$	
Stabilization Energy (kcal/mol)	1	-24.75	
	3	-24.75	
	5	14.69	
Spin Density ($e/a.u^3$), Spin polarization parameter (ζ) and spin density plot	1	$(B_{encap})_1=1.00$ $(B_{encap})_2=-1.00$ $\zeta=0.0$	
	3	$(B_{encap})_1=1.00$ $(B_{encap})_2=1.00$ $\zeta=1.0$	
Thermodynamic parameter (kcal/mol)	3	$\Delta G_{encapsulation} = -8.87$ $\Delta G_{dimerization} = 4.67$	$\Delta H_{encapsulation} = -23.55$ $\Delta H_{dimerization} = -13.42$
VIP (eV)	3	7.00	
VEA (eV)	3	-2.81	

Table S3 the molecular orbital (with an isodensity value of 0.02) and spin density distribution (with an isodensity value of 0.0004) plots of stable spin states of various endohedral heterofullerenes. The blue color represents the excess of α spin density, and the orange color represents the excess of β spin density.

		Singlet	Triplet
	Molecular Orbital	 α-HOMO β-HOMO	 α-HOMO α-HOMO-1
	Spin Density		
$(B@C_{59}N)_2$	Molecular Orbital	 α-HOMO β-HOMO	 α-HOMO α-HOMO-1
	Spin Density		

$\text{B@C}_{59}\text{N}-\text{N@C}_{59}\text{B}$		Singlet	Triplet	Quintet
	Molecular Orbital	 α-HOMO HOMO β-	 β-HOMO α-HOMO-60 α-HOMO-61 α-HOMO-62	 α-HOMO α-HOMO-60 α-HOMO-61 α-HOMO-62
$\text{B@C}_{59}\text{N}-\text{N@C}_{59}\text{B}$	Spin Density			

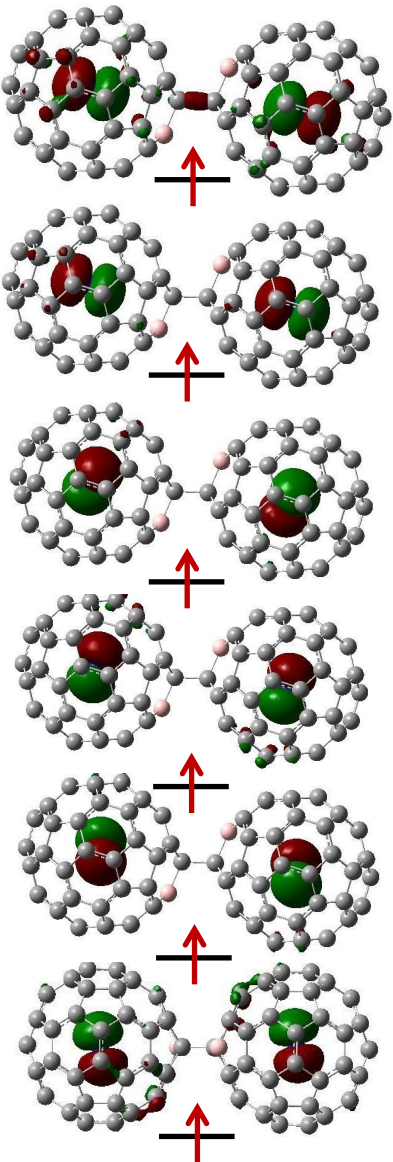
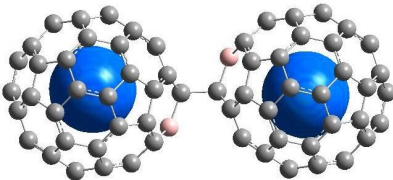
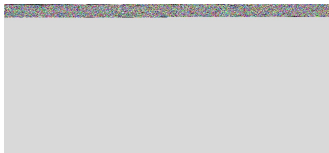
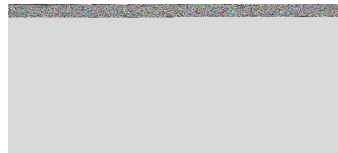
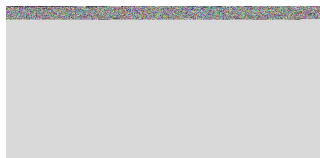
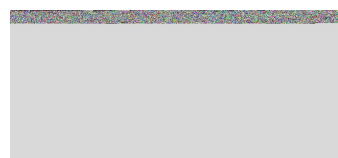
(N@C ₅₉ B) ₂	Septet	
	Molecular Orbitals	 α-HOMO-60 α-HOMO-61 α-HOMO-62 α-HOMO-63 α-HOMO-64 α-HOMO-65
	Spin Density	

Table S4 The calculated parameters of (B@C₅₉N)₂ at B3LYP-GD2 and B3LYP-GD3 functional using the basis set 6-311G*

	Multiplicity	B3LYP-GD2	B3LYP-GD3
Stabilization Energy (kcal/mol)	1	-24.23	-30.58
	3	-24.23	-30.58
	5	10.17	4.21
Spin Density (e/au ³), Spin polarization parameter (ζ) and spin density plot	1	$(B_{\text{encap}})_1=1.00$ $(B_{\text{encap}})_2=-1.00$ $(N_{\text{cage}})_1=(N_{\text{cage}})_2=0.00$ $\zeta=0.0$ 	$(B_{\text{encap}})_1=1.00$ $(B_{\text{encap}})_2=-1.00$ $(N_{\text{cage}})_1=(N_{\text{cage}})_2=0.00$ $\zeta=0.0$ 
	3	$(B_{\text{encap}})_1=1.00$ $(B_{\text{encap}})_2=1.00$ $(N_{\text{cage}})_1=(N_{\text{cage}})_2=0.00$ $\zeta=1.0$ 	$(B_{\text{encap}})_1=1.00$ $(B_{\text{encap}})_2=1.00$ $(N_{\text{cage}})_1=(N_{\text{cage}})_2=0.00$ $\zeta=1.0$ 
VIP (eV)	3	6.88	6.82
VEA (eV)	3	-2.77	-2.82

Cartesian coordinates of the optimized geometries

(C₅₉B)₂

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¹[(B@C₅₉B)₂]

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 C,1.2409081335,7.0659961981,-2.2981544015

³[(B@C₅₉B)₂]

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(C₅₉N)₂

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¹[(B@C₅₉N)₂]

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¹[B@C₅₉N-N@C₅₉B]

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⁵[B@C₅₉N-N@C₅₉B]

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